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STRONGLY COUPLED PLASMA RESEARCH FOR THE EQUATION OF STATE AND CONDUCTIVITY OF A LASER-COMPRESSED ELECTRON-ION PLASMA

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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

A novel scheme for the analysis of dense, strongly coupled plasmas, occurring in laser compression (and other) experiments, has been developed. The scheme has been applied to the analysis both of static and of dynamic properties of such plasmas. Comparison with conventional perturbative weak coupling theories and with other strong coupling schemes have been performed: they confirm the superiority of the present scheme.

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I. INTRODUCTION

In this Report we summarize the results and accomplishments of the work done on the analysis of strongly coupled plasmas systems. While such systems occur under a great variety of physical conditions and in many different physical systems, our work was motivated by the fact that laser compressed plasmas become strongly coupled (especially in the blow-off region). The strong coupling is expected to affect both equilibrium and non-equilibrium properties. Strong coupling results when the average potential energy of particles becomes comparable to or exceeds their kinetic energy. Its measure can be chosen as this latter ratio, $\Gamma = \frac{Z^2e^2}{dT}$ (here Ze is the ionic charge, d the average interparticle distance, and T the temperature or energy unit). An alternatively useful characterization of the system is through the parameter $\gamma = \frac{\kappa^3}{4\pi n} = \sqrt{3}\,\Gamma^{3/2}$ (here $\kappa = (4\pi e^2 Zn/T)^{1/2}$ is the DEBYE wave number). The domain of interest for strong coupling is evidently $\Gamma \gtrsim 1$, or $\gamma \gtrsim 1$.

II. HISTORICAL BACKGROUND

The crux of the theoretical problem involved in strongly coupled plasma research is to find a non-perturbative method which avoids the usual expansion in γ (or Γ), applicable to weakly coupled plasmas. Since the frequency- and wave-number-dependent dielectric function $\varepsilon(\underline{k}\omega)$ contains most of the information relevant to equilibrium and transport processes, a non-perturbative method that provides a calculation tool for the latter is the principal objective in this search. As early as 1967, Hubbard(1) suggested a method, which consisted of calculating $\varepsilon(\underline{k}\omega)$ from a kinetic equation, where the collision term in approximated by an expression involving only the static, equilibrium pair correlation function g(r), and then by using the fluctuation-dissipation theorem (FDT) to link $\varepsilon(\underline{k}0)$ to $g_{\underline{k}}$, thus providing a self-consistency requirement which leads to an integral equation for $g_{\underline{k}}$. Hubbard's method was substantially improved and worked out in great detail by Singwi, Tosi, Land, and

Sjolander[2] into a comprehensive structure, which has become to be known as the STLS theory. Other workers starting from different premises arrived at structures similar to STLS. Common to all these approaches is the notion of static effective potential, which replaces the Coulomb potential in $\varepsilon(\underline{k}\omega)$; otherwise $\varepsilon(\underline{k}\omega)$ has the same structure as in the Vlasov approximation. This feature points at the main defect of these "mean field theories": no genuine dynamical correlations and collisional effects was described by them.

It is obvious that what is needed to cure this defect is a more sophisticated approximation for the non-equilibrium two-body function. This was pointed out by Kalman in his 1972 Les Houches lectures.[3] The way to such an approach became accessible through an earlier (1972) work of Golden, Kalman, and Silevitch,[4] which provided a non-linear extension of the convectional linear FDT. In 1974 Golden, Kalman and Silevitch (GKS) published the outlines of a new approach to strongly coupled plasmas.[5] In the GKS theory, the non-equilibrium two-body function is approximated by its velocity average approximation, VAA). Using the nonlinear FDT, the resulting object can be related to the quadratic polarizability; thus, an expression for $\varepsilon(\underline{k}\omega)$ in terms of the quadratic polarizability is generated; self consistency is achieved by independently expressing the latter in terms of $\varepsilon(\underline{k}\omega)$.

III. CHRONOLOGICAL SUMMARY OF WORK

In order to handle electron-ion systems, first the generalization of the original one component (ocp) theories to two component situations was necessary. This was done in A (works done under the present Grant are listed by alphabetical code), where the two compenent static ($\omega=0$) form of the GKS and other theories was worked out. The divergence of the classical electron-ion pair correlation function was removed with the aid of a phenomonological "soft-core" potential. An important formal development of the work was the introduction of "partial" linear and nonlinear polarizabilities. The result of the analysis was the derivation of a set of three, coupled nonlinear integral equations for the pair correlations or polarizabilities.

One of the important strong coupling effects on electron-ion plasmas is the lowering of the ionization potential. In B we formulated a scheme to calculate this effect with the aid of the equilibrium pair correlation functions. These pair correlations can be calculated by numerically solving the nonlinear integral equations derived in A. The scheme, however, does not take account of the free-bound interaction, which is accessible only through a more detailed quantum mechanical calculation.

Two different lines of research were started in 1976, both aimed at clarifying the implications and defects of the various approximation schemes. The first approach consisted of studying the approximate equations for the pair correlation function in configuration space representation. The structure of the resulting integro-differential equation shows that for $r\to 0$ the pair correlation function in all the mean field theories exhibits a pathological behavior. A preliminary report on this investigation done in collaboration with M.B. Silevitch was given in C. A later work in 1977 (G) on the general properties of plasma corelation function is also an outgrowth of this activity.

The second approach compares known exact perturbative solutions for the pair correlation function and for $\epsilon(\underline{k}\omega)$ with $\gamma \to 0$ limits of the non-perturbative approximate solutions. A first attempt along this line in collaboration with M. Feix of the C.N.R.S., France and with M.B. Silevtich was given in D.

A continuation of the study of the depression of the ionization potential in strongly coupled plasmas was undertaken in collaboration with R. Engelman (of the Soreq Nuclear Research Center, Israel) in O. We examined the quantum mechanical basis of the phenomenological soft-core ion-electron potential and have derived the exact value of the free parameter in this phenomonological soft-core ion-electron potential and have derived the exact value of the free parameter in this phenomonological potential.

A very important criterion for all approximate $\epsilon(\underline{k}\omega)$ expressions is their high frequency behavior and their satisfaction of high frequency sum rules. In 1975 we derived (in collaboration with D. Merlini of the Ecole Federale de Polytechnique, Lausanne, Switzerland) a new sum rule for quadratic polarizabilities (while the usual sum rules pertain to the linear polarizabilities). We also investigated the GKS scheme from this point of view (Ref. E); the scheme was improved, so that the satisfaction of this particular sum rule was guaranteed. While this was possible for the GKS scheme, it was also shown that none of the other known approximation schemes can satisfy this sum rule.

A very fruitful line of research started in 1976-77, in collaboration with the group at the Ecole Federale de Polytechnique, Lausanne (Switzerland) concerning the properties of two-dimensional plasmas (with log r interaction). In addition to such situations occurring in nature, the two-dimensional plasma is an excellent theoretical laboratory where many problems, intractable in three dimensions, become soluble. Publication F (done in collaboration with D. Merlini of the EFP) derives

sum rules for such systems.

In 1976 the North Atlantic Treaty Organization awarded a grant to G. Kalman to organize a NATO Advanced Study Institute on the topic of Strongly Coupled Plasmas. The Institute was held in the summer of 1977 in Orleans-la-Source, France. Review papers presented at the Institute included one by G. Kalman on methods and approximations used in strongly coupled plasma research, (H), one by K.I. Golden on the use of response functions in theoretical schemes, and in the GKS scheme in particular, (I), and one by P. Bakshi on the configuration space approach to the strongly coupled plasma problem (J). The proceedings of the Institute were published in the volume "Strongly Coupled Plasmas" (K) which has become the central reference work in the field.

In the years 1978-79 in a series of works we continued the study of two-dimensional plasmas (L, M, N). We were able to derive an exact solution of the two-dimensional STLS integral equation for the pair-correlation function. For the first time, exact expressions valid for arbitrary coupling were derived for the correlation energy and the heat capacity. Detailed numerical studies of the correlation function both r- and k- representation were compared with the analytic formulae.

In the years 1976-78 a great deal of work was invested in the study of the numerical integration of the basic STLS integral equation (in three dimensions) for the pair correlation function, which has a structure similar to that of other schemes, including the GKS scheme. The equation has to be solved by a numerical iterative procedure. We have shown that the Debye-Huckel g_k cannot be used for the numerical interation scheme. A more satisfactory starting point is the solution of the "linearized" STLS equation, which includes correlations, but ignores collective effects. 4,000 gridpoints and quadratic Lagrangian interpolation methods

were used and interpolation was performed using Gaussian quadrature. Despite many efforts, in collaboration with M. Silevitch and B.A. Cover, then of KMS Fusion, Ann Arbor, the algorithm did not lead to adequate convergence, in contrast to the two-dimensional case, where convergence is obtained easily. We are now fairly certain that the kind of non-linear integral equation that features in the analysis is not amenable to iterative solution.

In the period 1978-79 we made significant progress (publications P and Q) in developing the crucially important dynamical (ω-dependent) version of the GKS theory. The development followed the earlier VAA approach, but went much further in the application of the nonlinear FDT to dynamical calculations. The resulting expression for $\alpha(\underline{k}\omega)$ (where $\varepsilon(\underline{k}\omega) = 1 + \alpha(\underline{k}\omega)$) is $\alpha(\underline{k}\omega) = \alpha_0(\underline{k}\omega)\{1 + v(\underline{k}\omega)\}$, where $\alpha_0(\underline{k}\omega)$ is the RPA polarizability and the dynamical screening function $v(\underline{k}\omega)$ is expressed in terms of quadratic polarizabilities. The dynamical expression is made self-consistent by a "dynamical superposition" scheme which consists of the decomposition of the quadratic polarizabilities in terms of linear polarizabilities: in the $k\to 0$ limit such a decomposition is exact for weak coupling. The result is a relatively simple integral equation for $\alpha(\underline{k}\omega)$. A method for the approximate solution of the integral equation was worked out in collaboration with P. Carini (R, S). A simple two-pole hydrodynamical model for the linear polarizability was adopted with the positions of the complex poles being treated as unknown parameters. This reduced the integral equation to an algebraic equation which then was numerically solved. The analysis, which is the first calculation of this kind, gave very good agreement with the molecular dynamics data of Hansen and collaborators for γ values up to crystallization ($\gamma \sim 3{,}200$). Paralleling the dynamical work we continued the comparison of the exact weak coupling results with the $\gamma\to 0$ limit of our calculations. To this end the dynamical perturbation analysis for $\varepsilon(\underline{k}\omega)$, done by Coste some time

ago,[(6)] was recalculated and numerically evaluated, using a new technique (Q, T, U). We found a good agreement with the plasmon dispersion in the $\gamma \to o$ limit. In particular, we have found that both calculations give decreasing $\frac{d\omega}{dk}$ slope with increasing γ. At the same time, we were puzzled to find some arguments in a paper by Ichimaru et al.[(7)] to the effect that the general strucutral requirements lead to $\frac{d\omega}{dk}$ increasing with increasing γ. On close examination the purported proof of Ichimaru et al. has turned out to be incorrect: this was discussed in publication V. Further work on the static weak coupling limit, concerning triplet and quadruplet correlations was done in collaboration with Y. Shima and H. Yatom of the Soreq Nuclear Research Center, Israel, in W. We used two approaches to obtain contributions through $O(\gamma^3)$. The first approach was through the conventional perturbation expansion of the BBGKY hierarchy; the second relies upon a chain of generalized non-linear FDT-s in terms of response functions of increasing nonlinearity.

In two recent papers (X and Y) we examined some of the general structural features and implications of the GKS theory. In X we use a moment expansion of the plasma kinetic equation to elucidate the meaning of the VAA. In Y we derived relationships for quadratic and cubic response functions and connected them with three- and four-point functions through generalized FDT relations. We introduced the novel concept of "response function of the second kind" relating to the perturbation of two-point functions. We also showed that the VAA is exact in the static limit. This observation allows one to combine experimentally and numerically obtained static data with the dynamical VAA scheme.

Also in the structural domain, but intended to extend the structural basis of the FDT formalism, are two works: Z and AA. Z develops the important extension of the nonlinear FDT to the quantum domain for degenerate plasmas, while AA discusses a mathematical problem, concerning derivatives of exponential operators, encountered in this development.

In 1980 we completed our numerical and analytic investigations of two dimensional plasma systems (BB): the equilibrium pair correlation function and the static $\varepsilon(\underline{k})$ were calculated in various approximations. The correlation energies obtained through different approximation schemes were compared and a good analytic fit, valid for arbitrary γ values, was found. We also studied some properties of surface plasmas (e.g. electron film on the surface of liquid He) in CC .

Of considerable practical importance is the understanding of the effect of strong coupling on various plasma instabilities. The most important amongst these is probably the beam-plasma instability. In 1980, in DD we examined the interaction of a low density electron beam with a high density strongly coupled plasma. Growth rate expressions were derived and the stability boundaries in parameter space were established.

Finally, over the years a number of invited conference presentations and talks were given by us at various international meetings: at the "Colloque sur les Systemes Coulombiens" in 1976 (EE), at the "N.C. Christopolos International Summer School" in 1977 (FF), at the "The Physics of Dense Matter" in 1979 (GG) and at the "International Conference on Recent Progress in Many Body Physics," in 1981 (HH).

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